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(2*E*)-1-(2-Hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one

B. K. Sarojini,[a] H. S. Yathirajan,[b] K. Mustafa,[a] H. Sarfraz[c] and Michael Bolte[d]*

[a]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, [b]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [c]Department of Physics, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and [d]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: bolte@chemie.uni-frankfurt.de

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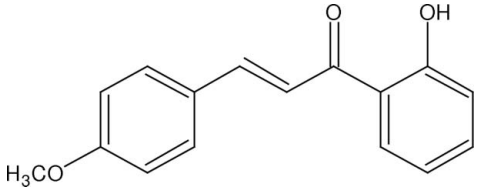
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.091; data-to-parameter ratio = 9.1.

Geometric parameters of the title compound, $C_{16}H_{14}O_3$, a chalcone derivative, are in the usual ranges. The C=C double bond is *trans* configured. The molecule is essentially planar (r.m.s. deviation for all non-H atoms = 0.066 Å). The molecular conformation is stabilized by an O—H···O hydrogen bond.

Related literature

For related literature, see: Butcher *et al.* (2007); Conti (2006); Domínguez *et al.* (2005); Fischer *et al.* (2007); Goto *et al.* (1991); Harrison *et al.* (2006); Indira *et al.* (2002); Lawrence *et al.* (2001); Nielsen *et al.* (2005); Pandey *et al.* (2005); Sarker & Nahar (2004); Sarojini *et al.* (2006); Yathirajan, Mayekar, Narayana *et al.* (2007); Yathirajan, Mayekar, Sarojini *et al.* (2007).



Experimental

Crystal data

$C_{16}H_{14}O_3$
M_r = 254.27
Orthorhombic, $Pca2_1$
a = 25.4158 (15) Å
b = 3.9662 (3) Å
c = 12.6046 (10) Å
V = 1270.60 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (2) K
0.41 × 0.37 × 0.36 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
15514 measured reflections
1624 independent reflections
1503 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.092
S = 1.07
1624 reflections
178 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*O*···O1	0.94 (3)	1.66 (3)	2.529 (2)	151 (3)

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2447).

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supplementary materials

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(2*E*)-1-(2-Hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one

B. K. Sarojini, H. S. Yathirajan, K. Mustafa, H. Sarfraz and M. Bolte

Comment

Chalcones are a class of naturally occurring compounds with wide spectrum of biological activities. Chalcones can be easily obtained from the aldol condensation of aromatic aldehydes and aromatic ketones. This class of compounds presents interesting biological properties such as cytotoxicity (Pandey *et al.*, 2005) and antiherpes activity and antitumour activity (Conti, 2006) and may be useful for the chemotherapy of leishmaniasis among others (Lawrence *et al.*, 2001). Chalcone derivatives are also used as antibiotics (Nielsen *et al.*, 2005) and as anti malerials (Domínguez *et al.*, 2005). A natural medicine genus Angelica is known to contain large number of naturally occurring chalcones (Sarker & Nahar, 2004). Chalcone derivatives are recognized for NLO properties and have good crystallization ability (Goto *et al.*, 1991; Indira *et al.*, 2002; Sarojini *et al.*, 2006). Structures of few related chalcones *viz*., (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxy-3-methoxyphenyl)prop-2-en-1-one (Yathirajan, Mayekar, Narayana *et al.*, 2007), (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxyphenyl)prop-2-en-1-one (Yathirajan, Mayekar, Sarojini *et al.*, 2007), 3-[4-(methylsulfanyl)phenyl]-1-(4-nitrophenyl)prop-2-en-1-one (Harrison *et al.*, 2006), 2E)-1-(3-hydroxyphenyl)-3-(4-methylphenyl)prop-2-en-1-one (Butcher *et al.*, 2007), (2E)-3-(biphenyl-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (Fischer *et al.*, 2007). In continuation of our studies on chalcones, a new chalcone is synthesized and its crystal structure is reported.

Geometric parameters of the title compound are in the usual ranges. The C—C double bond is *trans* configured. The molecule is essentially planar [r.m.s. deviation for all non-H atoms 0.066 Å]. The molecular conformation is stabilized by a O—H···O hydrogen bond.

Experimental

To a solution of 2-hydroxyacetophenone (1.36 g, 0.01 mol) and 4-methoxybenzaldehyde (1.36 g, 0.01 mol) in 25 ml e thanol, 50% KOH (2.5 ml) was added at 273 K. The mixture was stirred overnight at room temperature and then poured onto ice water. The pH of this mixture was adjusted to 3–4 with 2 *M* HCl aqueous solution. A yellow precipitate was collected by filtration and purified by recrystallization in ethanol. The single crystals were grown from acetone by slow evaporation method [m.p.: 343–348 K]. Analysis for $C_{16}H_{14}O_3$: Found (Calculated): C 75.63 (75.57), H 5.57% (5.55%).

Refinement

All H atoms were found in a difference map, but those bonded to C were geometrically positioned and refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C) or U(H) = 1.5 $U_{eq}(C_{methyl})$] using a riding model with C—H = 0.95 Å or 0.98 Å for $C_{aromatic}$—H and C_{methyl}—H, respectively. The methyl group was allowed to rotate but not to tip. The hydroxyl H atom was freely refined.

Figures

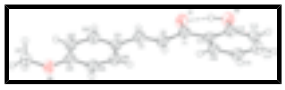

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

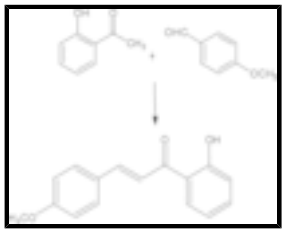

Fig. 2. The formation of the title compound.

(2E)-1-(2-Hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{14}O_3$	F_{000} = 536
M_r = 254.27	D_x = 1.329 Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 15446 reflections
a = 25.4158 (15) Å	θ = 2.4–28.5º
b = 3.9662 (3) Å	μ = 0.09 mm^{-1}
c = 12.6046 (10) Å	T = 173 (2) K
V = 1270.60 (16) Å^3	Block, yellow
Z = 4	0.41 × 0.37 × 0.36 mm

Data collection

Stoe IPDSII two-circle diffractometer	1503 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.079
Monochromator: graphite	θ_{max} = 28.2º
T = 173(2) K	θ_{min} = 2.3º
ω scans	h = −33→30
Absorption correction: none	k = −5→5
15514 measured reflections	l = −16→16
1624 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.036	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.092	$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
1624 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
178 parameters	$\Delta\rho_{min} = -0.17$ e Å^{-3}
1 restraint	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.039 (7)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.70169 (5)	0.6375 (4)	0.06637 (10)	0.0467 (3)
O2	0.79198 (6)	0.8269 (4)	0.00672 (10)	0.0481 (3)
H2O	0.7584 (14)	0.728 (7)	0.007 (3)	0.072 (8)*
O3	0.45867 (5)	0.2359 (3)	0.50165 (10)	0.0446 (3)
C1	0.70874 (7)	0.7522 (4)	0.15759 (14)	0.0370 (3)
C2	0.66887 (7)	0.7011 (4)	0.24036 (13)	0.0391 (4)
H2	0.6747	0.7888	0.3095	0.047*
C3	0.62427 (6)	0.5316 (4)	0.21939 (14)	0.0382 (4)
H3	0.6203	0.4512	0.1489	0.046*
C11	0.75813 (6)	0.9345 (4)	0.18289 (12)	0.0356 (3)
C12	0.79809 (7)	0.9589 (5)	0.10509 (13)	0.0386 (4)
C13	0.84559 (7)	1.1199 (5)	0.12829 (15)	0.0441 (4)
H13	0.8724	1.1336	0.0759	0.053*
C14	0.85365 (8)	1.2593 (4)	0.22747 (16)	0.0443 (4)
H14	0.8861	1.3679	0.2428	0.053*
C15	0.81458 (8)	1.2424 (5)	0.30568 (15)	0.0419 (4)
H15	0.8203	1.3404	0.3735	0.050*
C16	0.76767 (7)	1.0818 (5)	0.28309 (13)	0.0383 (4)
H16	0.7412	1.0702	0.3362	0.046*
C21	0.58134 (6)	0.4570 (4)	0.29245 (12)	0.0366 (3)
C22	0.53658 (7)	0.2907 (4)	0.25529 (13)	0.0396 (4)
H22	0.5349	0.2281	0.1826	0.048*
C23	0.49439 (7)	0.2138 (4)	0.32126 (14)	0.0391 (4)
H23	0.4641	0.1036	0.2938	0.047*

C24	0.49723 (7)	0.3013 (4)	0.42859 (13)	0.0370 (3)
C25	0.54173 (7)	0.4687 (5)	0.46771 (14)	0.0404 (4)
H25	0.5434	0.5307	0.5404	0.048*
C26	0.58315 (7)	0.5436 (4)	0.40097 (14)	0.0390 (4)
H26	0.6133	0.6550	0.4285	0.047*
C27	0.41243 (7)	0.0677 (5)	0.46422 (16)	0.0443 (4)
H27A	0.3965	0.1995	0.4068	0.066*
H27B	0.3872	0.0449	0.5226	0.066*
H27C	0.4219	−0.1565	0.4377	0.066*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0402 (6)	0.0677 (9)	0.0323 (5)	−0.0018 (6)	0.0003 (5)	−0.0049 (6)
O2	0.0422 (7)	0.0725 (8)	0.0294 (6)	−0.0016 (6)	0.0050 (5)	0.0000 (6)
O3	0.0356 (6)	0.0602 (8)	0.0381 (6)	−0.0025 (5)	0.0047 (5)	0.0017 (6)
C1	0.0348 (8)	0.0457 (8)	0.0305 (7)	0.0029 (6)	−0.0015 (6)	0.0016 (6)
C2	0.0342 (8)	0.0490 (9)	0.0341 (8)	0.0016 (6)	0.0005 (6)	0.0009 (7)
C3	0.0371 (8)	0.0445 (8)	0.0332 (7)	0.0016 (6)	0.0002 (6)	0.0001 (6)
C11	0.0326 (8)	0.0441 (8)	0.0300 (7)	0.0029 (6)	0.0006 (6)	0.0041 (6)
C12	0.0379 (8)	0.0479 (9)	0.0299 (7)	0.0029 (7)	0.0012 (6)	0.0053 (6)
C13	0.0376 (8)	0.0551 (10)	0.0396 (9)	−0.0004 (8)	0.0062 (7)	0.0082 (8)
C14	0.0371 (9)	0.0486 (9)	0.0473 (10)	−0.0032 (6)	−0.0028 (7)	0.0035 (7)
C15	0.0397 (8)	0.0475 (8)	0.0386 (8)	0.0010 (7)	−0.0032 (7)	−0.0008 (7)
C16	0.0376 (8)	0.0444 (8)	0.0329 (7)	0.0027 (6)	0.0007 (6)	0.0015 (6)
C21	0.0329 (7)	0.0426 (8)	0.0341 (8)	0.0014 (6)	−0.0012 (6)	0.0014 (6)
C22	0.0393 (8)	0.0475 (8)	0.0320 (7)	−0.0010 (7)	−0.0011 (6)	−0.0015 (7)
C23	0.0355 (8)	0.0458 (8)	0.0360 (8)	−0.0015 (6)	−0.0006 (7)	−0.0007 (7)
C24	0.0326 (8)	0.0436 (7)	0.0348 (8)	0.0026 (6)	0.0006 (6)	0.0027 (6)
C25	0.0350 (8)	0.0531 (9)	0.0329 (7)	0.0021 (7)	−0.0009 (6)	−0.0014 (7)
C26	0.0336 (8)	0.0477 (8)	0.0356 (7)	−0.0017 (6)	−0.0029 (6)	−0.0014 (7)
C27	0.0350 (8)	0.0500 (9)	0.0479 (9)	−0.0027 (7)	0.0048 (7)	0.0024 (8)

Geometric parameters (Å, °)

O1—C1	1.249 (2)	C14—H14	0.9500
O2—C12	1.355 (2)	C15—C16	1.381 (3)
O2—H2O	0.94 (3)	C15—H15	0.9500
O3—C24	1.370 (2)	C16—H16	0.9500
O3—C27	1.431 (2)	C21—C22	1.396 (2)
C1—C2	1.468 (2)	C21—C26	1.411 (2)
C1—C11	1.483 (2)	C22—C23	1.391 (2)
C2—C3	1.344 (2)	C22—H22	0.9500
C2—H2	0.9500	C23—C24	1.398 (2)
C3—C21	1.458 (2)	C23—H23	0.9500
C3—H3	0.9500	C24—C25	1.401 (2)
C11—C16	1.413 (2)	C25—C26	1.380 (2)
C11—C12	1.415 (2)	C25—H25	0.9500
C12—C13	1.397 (3)	C26—H26	0.9500

C13—C14	1.382 (3)	C27—H27A	0.9800
C13—H13	0.9500	C27—H27B	0.9800
C14—C15	1.401 (3)	C27—H27C	0.9800
C12—O2—H2O	105.4 (19)	C15—C16—H16	119.2
C24—O3—C27	117.02 (14)	C11—C16—H16	119.2
O1—C1—C2	120.31 (16)	C22—C21—C26	117.82 (15)
O1—C1—C11	119.78 (16)	C22—C21—C3	119.59 (14)
C2—C1—C11	119.90 (15)	C26—C21—C3	122.59 (15)
C3—C2—C1	120.75 (15)	C23—C22—C21	122.09 (15)
C3—C2—H2	119.6	C23—C22—H22	119.0
C1—C2—H2	119.6	C21—C22—H22	119.0
C2—C3—C21	127.47 (16)	C22—C23—C24	118.96 (16)
C2—C3—H3	116.3	C22—C23—H23	120.5
C21—C3—H3	116.3	C24—C23—H23	120.5
C16—C11—C12	117.90 (15)	O3—C24—C23	124.50 (15)
C16—C11—C1	122.63 (15)	O3—C24—C25	115.52 (14)
C12—C11—C1	119.46 (15)	C23—C24—C25	119.98 (16)
O2—C12—C13	117.86 (16)	C26—C25—C24	120.22 (15)
O2—C12—C11	121.71 (16)	C26—C25—H25	119.9
C13—C12—C11	120.44 (16)	C24—C25—H25	119.9
C14—C13—C12	120.02 (17)	C25—C26—C21	120.91 (16)
C14—C13—H13	120.0	C25—C26—H26	119.5
C12—C13—H13	120.0	C21—C26—H26	119.5
C13—C14—C15	120.82 (17)	O3—C27—H27A	109.5
C13—C14—H14	119.6	O3—C27—H27B	109.5
C15—C14—H14	119.6	H27A—C27—H27B	109.5
C16—C15—C14	119.26 (16)	O3—C27—H27C	109.5
C16—C15—H15	120.4	H27A—C27—H27C	109.5
C14—C15—H15	120.4	H27B—C27—H27C	109.5
C15—C16—C11	121.55 (16)		
O1—C1—C2—C3	−0.2 (3)	C12—C11—C16—C15	−0.6 (2)
C11—C1—C2—C3	−178.87 (16)	C1—C11—C16—C15	178.22 (17)
C1—C2—C3—C21	179.38 (15)	C2—C3—C21—C22	176.94 (18)
O1—C1—C11—C16	177.43 (16)	C2—C3—C21—C26	−3.7 (3)
C2—C1—C11—C16	−3.9 (2)	C26—C21—C22—C23	0.8 (3)
O1—C1—C11—C12	−3.7 (3)	C3—C21—C22—C23	−179.84 (15)
C2—C1—C11—C12	174.95 (14)	C21—C22—C23—C24	−1.0 (3)
C16—C11—C12—O2	−179.46 (15)	C27—O3—C24—C23	−0.3 (2)
C1—C11—C12—O2	1.7 (2)	C27—O3—C24—C25	179.49 (15)
C16—C11—C12—C13	0.9 (2)	C22—C23—C24—O3	−179.20 (15)
C1—C11—C12—C13	−177.94 (15)	C22—C23—C24—C25	1.0 (3)
O2—C12—C13—C14	179.82 (17)	O3—C24—C25—C26	179.33 (15)
C11—C12—C13—C14	−0.6 (3)	C23—C24—C25—C26	−0.9 (3)
C12—C13—C14—C15	−0.2 (3)	C24—C25—C26—C21	0.7 (3)
C13—C14—C15—C16	0.5 (3)	C22—C21—C26—C25	−0.6 (3)
C14—C15—C16—C11	−0.1 (3)	C3—C21—C26—C25	−179.97 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2O···O1	0.94 (3)	1.66 (3)	2.529 (2)	151 (3)

Fig. 1

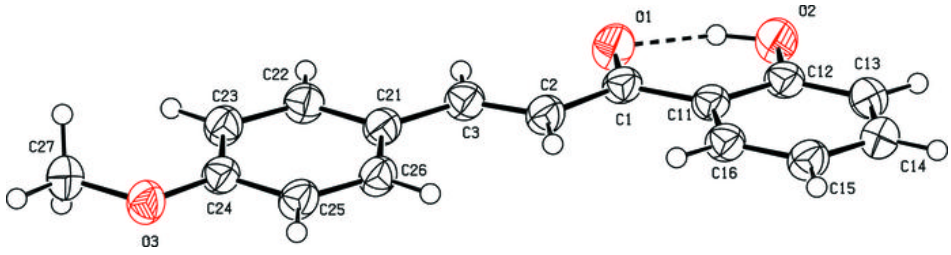
O1
O2
C22
C23
C21
C2
C12
C13
C27
C3
C1
C11
C26
C16
C14
C24
C25
C15
O3

Fig. 2